

Integrative Structure Validation Report

August 15, 2024 - 01:55 PM PDT

The following software was used in the production of this report:


Python-IHM Version 1.3

Integrative Modeling Validation Version 1.2

PDB ID	9A8L
PDB-Dev ID	PDBDEV_00000385
Structure Title	Modeling of Mouse NPC basket
Structure Authors	Singh, D.; Soni, N.; Hutchings, J.; Echeverria, I.; Shaikh, F.; Duquette, M.; Suslov, S.; Li, Z.; van Eeuwen, T.; Molloy, K.; Shi, Y.; Wang, J.; Guo, Q.; Chait, B.T.; Fernandez-Martinez, J.; Rout, M.P.; Sali, A.; Villa, E.

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

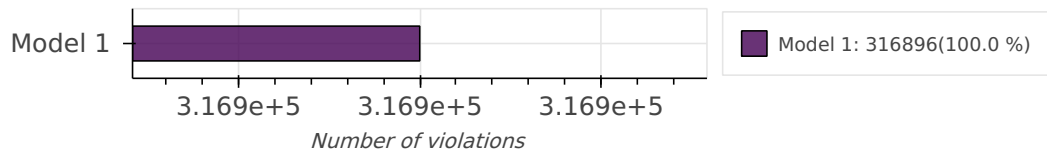
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the  symbol.

List of references used to build this report is available [here](#).

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis



Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 192 subunits in each model. A total of 6 datasets or restraints were used to build this entry. Each model is represented by 592 rigid bodies and 432 flexible or non-rigid units.

Entry composition ?

There is 1 unique type of models in this entry. This model is titled Cluster 0/centroid-C8-symmetric.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Nucleoprotein TPR	A	A	2431
1	2	1	Nucleoprotein TPR	B	B	2431
1	3	1	Nucleoprotein TPR	C	C	2431
1	4	1	Nucleoprotein TPR	D	D	2431
1	5	1	Nucleoprotein TPR	E	E	2431
1	6	1	Nucleoprotein TPR	F	F	2431
1	7	1	Nucleoprotein TPR	G	G	2431
1	8	1	Nucleoprotein TPR	H	H	2431
1	9	1	Nucleoprotein TPR	I	I	2431
1	10	1	Nucleoprotein TPR	J	J	2431
1	11	1	Nucleoprotein TPR	K	K	2431

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	12	1	Nucleoprotein TPR	L	L	2431
1	13	1	Nucleoprotein TPR	M	M	2431
1	14	1	Nucleoprotein TPR	N	N	2431
1	15	1	Nucleoprotein TPR	O	O	2431
1	16	1	Nucleoprotein TPR	P	P	2431
1	17	2	Nuclear pore complex protein Nup50	Q	Q	466
1	18	2	Nuclear pore complex protein Nup50	R	R	466
1	19	2	Nuclear pore complex protein Nup50	S	S	466
1	20	2	Nuclear pore complex protein Nup50	T	T	466
1	21	2	Nuclear pore complex protein Nup50	U	U	466
1	22	2	Nuclear pore complex protein Nup50	V	V	466
1	23	2	Nuclear pore complex protein Nup50	W	W	466
1	24	2	Nuclear pore complex protein Nup50	X	X	466
1	25	2	Nuclear pore complex protein Nup50	Y	Y	466
1	26	2	Nuclear pore complex protein Nup50	Z	Z	466
1	27	2	Nuclear pore complex protein Nup50	AA	AA	466
1	28	2	Nuclear pore complex protein Nup50	AB	AB	466

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	29	2	Nuclear pore complex protein Nup50	AC	AC	466
1	30	2	Nuclear pore complex protein Nup50	AD	AD	466
1	31	2	Nuclear pore complex protein Nup50	AE	AE	466
1	32	2	Nuclear pore complex protein Nup50	AF	AF	466
1	33	3	Nucleoporin 153	AG	AG	1462
1	34	3	Nucleoporin 153	AH	AH	1462
1	35	3	Nucleoporin 153	AI	AI	1462
1	36	3	Nucleoporin 153	AJ	AJ	1462
1	37	3	Nucleoporin 153	AK	AK	1462
1	38	3	Nucleoporin 153	AL	AL	1462
1	39	3	Nucleoporin 153	AM	AM	1462
1	40	3	Nucleoporin 153	AN	AN	1462
1	41	3	Nucleoporin 153	AO	AO	1462
1	42	3	Nucleoporin 153	AP	AP	1462
1	43	3	Nucleoporin 153	AQ	AQ	1462
1	44	3	Nucleoporin 153	AR	AR	1462
1	45	3	Nucleoporin 153	AS	AS	1462
1	46	3	Nucleoporin 153	AT	AT	1462
1	47	3	Nucleoporin 153	AU	AU	1462
1	48	3	Nucleoporin 153	AV	AV	1462

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	49	4	Nuclear pore complex protein Nup160	AW	AW	1402
1	50	4	Nuclear pore complex protein Nup160	AX	AX	1402
1	51	4	Nuclear pore complex protein Nup160	AY	AY	1402
1	52	4	Nuclear pore complex protein Nup160	AZ	AZ	1402
1	53	4	Nuclear pore complex protein Nup160	BA	BA	1402
1	54	4	Nuclear pore complex protein Nup160	BB	BB	1402
1	55	4	Nuclear pore complex protein Nup160	BC	BC	1402
1	56	4	Nuclear pore complex protein Nup160	BD	BD	1402
1	57	4	Nuclear pore complex protein Nup160	BE	BE	1402
1	58	4	Nuclear pore complex protein Nup160	BF	BF	1402
1	59	4	Nuclear pore complex protein Nup160	BG	BG	1402
1	60	4	Nuclear pore complex protein Nup160	BH	BH	1402
1	61	4	Nuclear pore complex protein Nup160	BI	BI	1402
1	62	4	Nuclear pore complex protein Nup160	BJ	BJ	1402
1	63	4	Nuclear pore complex protein Nup160	BK	BK	1402

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	64	4	Nuclear pore complex protein Nup160	BL	BL	1402
1	65	5	Nuclear pore complex protein Nup85	BM	BM	656
1	66	5	Nuclear pore complex protein Nup85	BN	BN	656
1	67	5	Nuclear pore complex protein Nup85	BO	BO	656
1	68	5	Nuclear pore complex protein Nup85	BP	BP	656
1	69	5	Nuclear pore complex protein Nup85	BQ	BQ	656
1	70	5	Nuclear pore complex protein Nup85	BR	BR	656
1	71	5	Nuclear pore complex protein Nup85	BS	BS	656
1	72	5	Nuclear pore complex protein Nup85	BT	BT	656
1	73	5	Nuclear pore complex protein Nup85	BU	BU	656
1	74	5	Nuclear pore complex protein Nup85	BV	BV	656
1	75	5	Nuclear pore complex protein Nup85	BW	BW	656
1	76	5	Nuclear pore complex protein Nup85	BX	BX	656
1	77	5	Nuclear pore complex protein Nup85	BY	BY	656
1	78	5	Nuclear pore complex protein Nup85	BZ	BZ	656

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	79	5	Nuclear pore complex protein Nup85	CA	CA	656
1	80	5	Nuclear pore complex protein Nup85	CB	CB	656
1	81	6	Nuclear pore complex protein Nup98-Nup96	CC	CC	1816
1	82	6	Nuclear pore complex protein Nup98-Nup96	CD	CD	1816
1	83	6	Nuclear pore complex protein Nup98-Nup96	CE	CE	1816
1	84	6	Nuclear pore complex protein Nup98-Nup96	CF	CF	1816
1	85	6	Nuclear pore complex protein Nup98-Nup96	CG	CG	1816
1	86	6	Nuclear pore complex protein Nup98-Nup96	CH	CH	1816
1	87	6	Nuclear pore complex protein Nup98-Nup96	CI	CI	1816
1	88	6	Nuclear pore complex protein Nup98-Nup96	CJ	CJ	1816
1	89	6	Nuclear pore complex protein Nup98-Nup96	CK	CK	1816
1	90	6	Nuclear pore complex protein Nup98-Nup96	CL	CL	1816
1	91	6	Nuclear pore complex protein Nup98-Nup96	CM	CM	1816
1	92	6	Nuclear pore complex protein Nup98-Nup96	CN	CN	1816
1	93	6	Nuclear pore complex protein Nup98-Nup96	CO	CO	1816

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	94	6	Nuclear pore complex protein Nup98-Nup96	CP	CP	1816
1	95	6	Nuclear pore complex protein Nup98-Nup96	CQ	CQ	1816
1	96	6	Nuclear pore complex protein Nup98-Nup96	CR	CR	1816
1	97	7	Protein SEC13 homolog	CS	CS	322
1	98	7	Protein SEC13 homolog	CT	CT	322
1	99	7	Protein SEC13 homolog	CU	CU	322
1	100	7	Protein SEC13 homolog	CV	CV	322
1	101	7	Protein SEC13 homolog	CW	CW	322
1	102	7	Protein SEC13 homolog	CX	CX	322
1	103	7	Protein SEC13 homolog	CY	CY	322
1	104	7	Protein SEC13 homolog	CZ	CZ	322
1	105	7	Protein SEC13 homolog	DA	DA	322
1	106	7	Protein SEC13 homolog	DB	DB	322
1	107	7	Protein SEC13 homolog	DC	DC	322
1	108	7	Protein SEC13 homolog	DD	DD	322
1	109	7	Protein SEC13 homolog	DE	DE	322
1	110	7	Protein SEC13 homolog	DF	DF	322
1	111	7	Protein SEC13 homolog	DG	DG	322
1	112	7	Protein SEC13 homolog	DH	DH	322
1	113	8	Nucleoporin SEH1	DI	DI	360
1	114	8	Nucleoporin SEH1	DJ	DJ	360

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	115	8	Nucleoporin SEH1	DK	DK	360
1	116	8	Nucleoporin SEH1	DL	DL	360
1	117	8	Nucleoporin SEH1	DM	DM	360
1	118	8	Nucleoporin SEH1	DN	DN	360
1	119	8	Nucleoporin SEH1	DO	DO	360
1	120	8	Nucleoporin SEH1	DP	DP	360
1	121	8	Nucleoporin SEH1	DQ	DQ	360
1	122	8	Nucleoporin SEH1	DR	DR	360
1	123	8	Nucleoporin SEH1	DS	DS	360
1	124	8	Nucleoporin SEH1	DT	DT	360
1	125	8	Nucleoporin SEH1	DU	DU	360
1	126	8	Nucleoporin SEH1	DV	DV	360
1	127	8	Nucleoporin SEH1	DW	DW	360
1	128	8	Nucleoporin SEH1	DX	DX	360
1	129	9	Nuclear pore complex protein Nup107	DY	DY	926
1	130	9	Nuclear pore complex protein Nup107	DZ	DZ	926
1	131	9	Nuclear pore complex protein Nup107	EA	EA	926
1	132	9	Nuclear pore complex protein Nup107	EB	EB	926
1	133	9	Nuclear pore complex protein Nup107	EC	EC	926

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	134	9	Nuclear pore complex protein Nup107	ED	ED	926
1	135	9	Nuclear pore complex protein Nup107	EE	EE	926
1	136	9	Nuclear pore complex protein Nup107	EF	EF	926
1	137	9	Nuclear pore complex protein Nup107	EG	EG	926
1	138	9	Nuclear pore complex protein Nup107	EH	EH	926
1	139	9	Nuclear pore complex protein Nup107	EI	EI	926
1	140	9	Nuclear pore complex protein Nup107	EJ	EJ	926
1	141	9	Nuclear pore complex protein Nup107	EK	EK	926
1	142	9	Nuclear pore complex protein Nup107	EL	EL	926
1	143	9	Nuclear pore complex protein Nup107	EM	EM	926
1	144	9	Nuclear pore complex protein Nup107	EN	EN	926
1	145	10	Nuclear pore complex protein Nup133	EO	EO	1155
1	146	10	Nuclear pore complex protein Nup133	EP	EP	1155
1	147	10	Nuclear pore complex protein Nup133	EQ	EQ	1155
1	148	10	Nuclear pore complex protein Nup133	ER	ER	1155

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	149	10	Nuclear pore complex protein Nup133	ES	ES	1155
1	150	10	Nuclear pore complex protein Nup133	ET	ET	1155
1	151	10	Nuclear pore complex protein Nup133	EU	EU	1155
1	152	10	Nuclear pore complex protein Nup133	EV	EV	1155
1	153	10	Nuclear pore complex protein Nup133	EW	EW	1155
1	154	10	Nuclear pore complex protein Nup133	EX	EX	1155
1	155	10	Nuclear pore complex protein Nup133	EY	EY	1155
1	156	10	Nuclear pore complex protein Nup133	EZ	EZ	1155
1	157	10	Nuclear pore complex protein Nup133	FA	FA	1155
1	158	10	Nuclear pore complex protein Nup133	FB	FB	1155
1	159	10	Nuclear pore complex protein Nup133	FC	FC	1155
1	160	10	Nuclear pore complex protein Nup133	FD	FD	1155
1	161	11	Nucleoporin Nup37	FE	FE	326
1	162	11	Nucleoporin Nup37	FF	FF	326
1	163	11	Nucleoporin Nup37	FG	FG	326
1	164	11	Nucleoporin Nup37	FH	FH	326
1	165	11	Nucleoporin Nup37	FI	FI	326

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	166	11	Nucleoporin Nup37	FJ	FJ	326
1	167	11	Nucleoporin Nup37	FK	FK	326
1	168	11	Nucleoporin Nup37	FL	FL	326
1	169	11	Nucleoporin Nup37	FM	FM	326
1	170	11	Nucleoporin Nup37	FN	FN	326
1	171	11	Nucleoporin Nup37	FO	FO	326
1	172	11	Nucleoporin Nup37	FP	FP	326
1	173	11	Nucleoporin Nup37	FQ	FQ	326
1	174	11	Nucleoporin Nup37	FR	FR	326
1	175	11	Nucleoporin Nup37	FS	FS	326
1	176	11	Nucleoporin Nup37	FT	FT	326
1	177	12	Nucleoporin Nup43	FU	FU	380
1	178	12	Nucleoporin Nup43	FV	FV	380
1	179	12	Nucleoporin Nup43	FW	FW	380
1	180	12	Nucleoporin Nup43	FX	FX	380
1	181	12	Nucleoporin Nup43	FY	FY	380
1	182	12	Nucleoporin Nup43	FZ	FZ	380
1	183	12	Nucleoporin Nup43	GA	GA	380
1	184	12	Nucleoporin Nup43	GB	GB	380
1	185	12	Nucleoporin Nup43	GC	GC	380
1	186	12	Nucleoporin Nup43	GD	GD	380
1	187	12	Nucleoporin Nup43	GE	GE	380
1	188	12	Nucleoporin Nup43	GF	GF	380

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	189	12	Nucleoporin Nup43	GG	GG	380
1	190	12	Nucleoporin Nup43	GH	GH	380
1	191	12	Nucleoporin Nup43	GI	GI	380
1	192	12	Nucleoporin Nup43	GJ	GJ	380

Datasets used for modeling

There are 6 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	De Novo model	File	10.5281/zenodo.13131753
3	Comparative model	File	10.5281/zenodo.13131753
5	3DEM volume	File	10.5281/zenodo.13131753
6	3DEM volume	File	10.5281/zenodo.13131753
2	Experimental model	PDB	7r5j
4	3DEM volume	EMDB	EMD-44379

Representation

This entry has only one representation and includes 592 rigid bodies and 432 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
AG	36-57	1-35, 58-428, 540-574
AH	36-57	1-35, 58-428, 540-574

Chain ID	Rigid bodies	Non-rigid segments
A	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
B	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
C	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
D	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
E	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
F	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431

Chain ID	Rigid bodies	Non-rigid segments
G	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
H	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
I	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
J	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
K	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
L	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431

Chain ID	Rigid bodies	Non-rigid segments
M	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
N	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
O	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
P	96-120, 124-180, 187-247, 254-285, 289-356, 360-405, 413-451, 511-595, 639-681, 757-883, 901-946, 947-999, 1004-1060, 1064-1106, 1107-1131, 1135-1163, 1170-1201, 1205-1254, 1281-1337, 1343-1420, 1424-1491, 1543-1616, 1627-1690	1-95, 121-123, 181-186, 248-253, 286-288, 357-359, 406-412, 452-510, 596-638, 682-756, 884-900, 1000-1003, 1061-1063, 1132-1134, 1164-1169, 1202-1204, 1255-1280, 1338-1342, 1421-1423, 1492-1542, 1617-1626, 1691-2431
Q	151-204, 355-466	1-150, 205-354
R	151-204, 355-466	1-150, 205-354
S	151-204, 355-466	1-150, 205-354
T	151-204, 355-466	1-150, 205-354
U	151-204, 355-466	1-150, 205-354
V	151-204, 355-466	1-150, 205-354
W	151-204, 355-466	1-150, 205-354
X	151-204, 355-466	1-150, 205-354
Y	151-204, 355-466	1-150, 205-354

Chain ID	Rigid bodies	Non-rigid segments
Z	151-204, 355-466	1-150, 205-354
AA	151-204, 355-466	1-150, 205-354
AB	151-204, 355-466	1-150, 205-354
AC	151-204, 355-466	1-150, 205-354
AD	151-204, 355-466	1-150, 205-354
AE	151-204, 355-466	1-150, 205-354
AF	151-204, 355-466	1-150, 205-354
AI	36-57	1-35, 58-428, 540-574
AJ	36-57	1-35, 58-428, 540-574
AK	36-57	1-35, 58-428, 540-574
AL	36-57	1-35, 58-428, 540-574
AM	36-57	1-35, 58-428, 540-574
AN	36-57	1-35, 58-428, 540-574
AO	36-57	1-35, 58-428, 540-574
AP	36-57	1-35, 58-428, 540-574
AQ	36-57	1-35, 58-428, 540-574
AR	36-57	1-35, 58-428, 540-574
AS	36-57	1-35, 58-428, 540-574
AT	36-57	1-35, 58-428, 540-574
AU	36-57	1-35, 58-428, 540-574
AV	36-57	1-35, 58-428, 540-574
AW	1-1402	-

Chain ID	Rigid bodies	Non-rigid segments
AX	1-1402	-
AY	1-1402	-
AZ	1-1402	-
BA	1-1402	-
BB	1-1402	-
BC	1-1402	-
BD	1-1402	-
BE	1-1402	-
BF	1-1402	-
BG	1-1402	-
BH	1-1402	-
BI	1-1402	-
BJ	1-1402	-
BK	1-1402	-
BL	1-1402	-
BM	1-656	-
BN	1-656	-
BO	1-656	-
BP	1-656	-
BQ	1-656	-
BR	1-656	-
BS	1-656	-
BT	1-656	-

Chain ID	Rigid bodies	Non-rigid segments
BU	1-656	-
BV	1-656	-
BW	1-656	-
BX	1-656	-
BY	1-656	-
BZ	1-656	-
CA	1-656	-
CB	1-656	-
CC	1111-1159, 1194-1816	-
CD	1111-1159, 1194-1816	-
CE	1111-1159, 1194-1816	-
CF	1111-1159, 1194-1816	-
CG	1111-1159, 1194-1816	-
CH	1111-1159, 1194-1816	-
CI	1111-1159, 1194-1816	-
CJ	1111-1159, 1194-1816	-
CK	1111-1159, 1194-1816	-
CL	1111-1159, 1194-1816	-
CM	1111-1159, 1194-1816	-
CN	1111-1159, 1194-1816	-
CO	1111-1159, 1194-1816	-
CP	1111-1159, 1194-1816	-
CQ	1111-1159, 1194-1816	-

Chain ID	Rigid bodies	Non-rigid segments
CR	1111-1159, 1194-1816	-
CS	1-302	-
CT	1-302	-
CU	1-302	-
CV	1-302	-
CW	1-302	-
CX	1-302	-
CY	1-302	-
CZ	1-302	-
DA	1-302	-
DB	1-302	-
DC	1-302	-
DD	1-302	-
DE	1-302	-
DF	1-302	-
DG	1-302	-
DH	1-302	-
DI	1-324	-
DJ	1-324	-
DK	1-324	-
DL	1-324	-
DM	1-324	-
DN	1-324	-

Chain ID	Rigid bodies	Non-rigid segments
DO	1-324	-
DP	1-324	-
DQ	1-324	-
DR	1-324	-
DS	1-324	-
DT	1-324	-
DU	1-324	-
DV	1-324	-
DW	1-324	-
DX	1-324	-
DY	145-926	-
DZ	145-926	-
EA	145-926	-
EB	145-926	-
EC	145-926	-
ED	145-926	-
EE	145-926	-
EF	145-926	-
EG	145-926	-
EH	145-926	-
EI	145-926	-
EJ	145-926	-
EK	145-926	-

Chain ID	Rigid bodies	Non-rigid segments
EL	145-926	-
EM	145-926	-
EN	145-926	-
EO	70-1155	-
EP	70-1155	-
EQ	70-1155	-
ER	70-1155	-
ES	70-1155	-
ET	70-1155	-
EU	70-1155	-
EV	70-1155	-
EW	70-1155	-
EX	70-1155	-
EY	70-1155	-
EZ	70-1155	-
FA	70-1155	-
FB	70-1155	-
FC	70-1155	-
FD	70-1155	-
FE	1-326	-
FF	1-326	-
FG	1-326	-
FH	1-326	-

Chain ID	Rigid bodies	Non-rigid segments
FI	1-326	-
FJ	1-326	-
FK	1-326	-
FL	1-326	-
FM	1-326	-
FN	1-326	-
FO	1-326	-
FP	1-326	-
FQ	1-326	-
FR	1-326	-
FS	1-326	-
FT	1-326	-
FU	1-292, 327-380	-
FV	1-292, 327-380	-
FW	1-292, 327-380	-
FX	1-292, 327-380	-
FY	1-292, 327-380	-
FZ	1-292, 327-380	-
GA	1-292, 327-380	-
GB	1-292, 327-380	-
GC	1-292, 327-380	-
GD	1-292, 327-380	-
GE	1-292, 327-380	-

Chain ID	Rigid bodies	Non-rigid segments
GF	1-292, 327-380	-
GG	1-292, 327-380	-
GH	1-292, 327-380	-
GI	1-292, 327-380	-
GJ	1-292, 327-380	-

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	500	False	True
2	1	Replica exchange monte carlo	Sampling	None	9569309	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.19.0	integrative model building	https://integrativemodeling.org
3	COCONUT	1.0.0	Coiled-coil model building	https://github.com/neeleshsoni21/COCONUT
2	Integrative Modeling Platform (IMP)	2.19.0	integrative model building	https://integrativemodeling.org

Data quality ?

3DEM volume

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobrity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below.

Models	Excluded Volume Satisfaction (%)	Number of violations
1	100.0	316896.0

Fit of model to data used for modeling ?

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

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